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The small polaron crossover: comparison between exact results and vertex correction approximation

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Abstract. – We study the crossover from quasi free electron to small polaron in the Holstein model for a single electron by means of both exact and self-consistent calculations in one dimension and on an infinite coordination lattice. We show that the crossover occurs when both strong coupling ($\lambda > 1$) and multiphonon ($\alpha^2 > 1$) conditions are fulfilled leading to different relevant coupling constants (λ) in adiabatic and (α^2) anti adiabatic region of the parameters space. We also show that the self-consistent calculations obtained by including the first electron-phonon vertex correction give accurate results in a sizeable region of the phase diagram well separated from the polaronic crossover.

Recent optical measurements of the insulating parent compounds of the high-temperature superconductors [1] show the presence of polaronic carriers, and evidence for strong electron-phonon (el-ph) coupling effects has been given also for the colossal magnetoresistance manganites [2] and Nickel compounds [3]. These findings underline the necessity of a clear theoretical description of electron-phonon coupled system and more specifically of the constraints for the existence of the small polaron ground state. This state, characterized by strong local electron-lattice correlation, is definitively a non-perturbative phenomenon, and cannot be described by simple summation of the perturbative series such as the one which defines the Migdal-Eliashberg (ME) theory [4, 5].

The aim of this work is to provide a detailed study of the crossover which occurs at intermediate electron-lattice couplings from quasi-free electron to small polaron ground state. We also study the role of the lattice dimensionality and compare exact results with self-consistent theories.

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A single electron interacting with Einstein phonons through an Holstein type local interaction is the simplest system which shows such kind of crossover. The associated hamiltonian is [6]:

$$\mathcal{H} = -t \sum_{\langle ij \rangle} c_i^\dagger c_j + g \sum_i n_i \left(a_i + a_i^\dagger \right) + \omega_0 \sum_i a_i^\dagger a_i \tag{1}$$

where c_i ($c_i^\dagger$) is the destruction (creation) operator for an electron on site i , and $n_i = c_i^\dagger c_i$. a_i ($a_i^\dagger$) is the destruction (creation) operator for Einstein dispersionless phonons with frequency ω_0 on site i. The hamiltonian (1) represents a non-trivial many-body problem even in the single electron case due to the quantum nature of phonons and it has been already studied in recent years by means of numerical [5, 7, 8, 9] and analytical [10, 11, 12] techniques.

For the hamiltonian of eq.(1) two dimensionless parameters, which measure the electron-lattice coupling, are introduced: $\lambda = g^2/(D\omega_0)$ and $\alpha = g/\omega_0$, where $D = 2td$ is the half-bandwidth for the free electron and d is the system dimensionality.

λ is originally introduced in the standard weak coupling pertubation theory ($g/t \ll 1$) and is the coupling parameter of a ME approach in the case of one electron. On the other hand λ is the ratio between the small polaron energy $E_{\rm p} = -g^2/\omega_0$ and the free electron energy $E_{\rm free} = -D$, so it naturally measures the energetic gain of the small polaron state with respect to the free electron-like state.

The parameter α is instead introduced in the standard small polaron theory and is also the relevant coupling in the *atomic limit* ($t = 0$). In this limit α measures the lattice displacement associated to the polaron and α^2 is the average number of phonons bound to the electron. According to the Lang-Firsov results [13] followed by the Holstein approximation[6] it also rules the reduction of the effective hopping $t^* = t \exp(-\alpha^2)$ [14, 15].

Besides λ and α, the el-ph system described by eq.(1) is governed also by another dimensionless parameter: ω_0/t. It measures the the degree of adiabaticy of the lattice motion (lattice kinetic energy $\simeq \omega_0$) compared to the electron one (electron kinetic energy $\simeq t$)([1]).

A bound state between electron and phonon is formed as soon as $\lambda > 1$. In the adiabatic regime ($\omega_0/t \ll 1$) this condition is sufficient to give a polaronic state since the electron is bound to the slowly moving lattice giving rise to a strong enhancement of effective mass. In the antiadiabatic regime ($\omega_0/t \gg 1$) such a picture is no longer true due to the fast lattice motion. In this case, polaronic features such as strong local electron-lattice correlations arise only when the electron is bound to a *large* number of phonons. This condition is fulfilled for $\alpha^2 > 1$. To summarize in both adiabatic and antiadiabatic regimes to have a polaronic state we must have *both* $\lambda > 1$ and $\alpha^2 > 1$ [14]. The above discussion stresses that $\lambda > 1$ is not the only condition for small polaron formation, in contrast with the claim of ref.[10].

The parameter ω_0/t influences also the dependence of the behavior of the el-ph coupled system on the system dimensionality. We shall show that in the antiadiabatic regime the constraint for the small polaron state is rather universal, *i. e.*, it does not depend on the system dimensionality. On the other hand, dimensionality plays an important role in the adiabatic limit $\omega_0/t = 0$. In fact, In d=1 the ground state is localized for any finite value of λ and a crossover occurs between large and small polaron around $\lambda \simeq 1$ whereas for $d \geq 2$ it has been shown that a localization transition occurs at finite λ from free electron to small polaron[16].

([1]) We stress that all the parameters we consider are defined in terms of the *bare* quantities t, ω_0 and g appearing in the hamiltonian (1).

The relevance of the adiabatic parameter ω_0/t and the role of dimensionality is exploited non perturbatively by using two alternative procedures, which both give exact numerical results:

i) Exact diagonalization of small one dimensional clusters by means of the Lanczos algorithm (ED-1d).

ii) Dynamical mean field theory (DMFT-3d).

In the exact diagonalization approach, the infinite phonon Hilbert space has to be truncated to allow for a given maximum number of phonons per site $n_{\max}$. In order to properly describe the multiphonon regime (expecially in the adiabatic regime where a large number of low energy phonons can be excited) our cut-off is $n_{\max} = 20$. This relatively high value forced us to restrict to a four-site cluster with periodic boundaries condition in the strong-coupling adiabatic regime. In the weak-coupling regime and for larger phonon frequencies a lower value of $n_{\max}$ is needed, allowing us to consider larger clusters up to ten sites. We checked that finite-size effects do not significantly affect the cross-over coupling, since small-polaron formation is a local, high energy process.

The dynamical mean field theory approach can be seen as the exact solution of the small polaron problem defined on an infinite coordination lattice. For this reason this theory does not suffer of limitations of other approach such as the variational [15] which may be in contraddiction with the Gerlach-Lowen theorem [17, 18]. The formulation of the DMFT requires the knowledge of the free particle DOS so that by choosing a semi-circular free particle DOS, it is possible to mimic a realistic three-dimensional case (DMFT-3d). Details of perturbation theory expansion in the DMFT framework are given in Ref. [11] together with results concerning the exact spectral properties.

Here, we study the behavior of the ground state energy E_0 using the exact solutions ED-1d and DMFT-3d and we compare the results with the self-consistent non-crossing (NCA) and vertex corrected approximations (VCA). These two approximations are defined by the self-consistent calculation of the electronic zero-temperature self-energy $\Sigma(k,\omega)$ given below:

$$\Sigma(k,\omega)=\frac{2\lambda\omega_0 t}{N}\sum_p G(p,\omega-\omega_0)\left[1+\frac{2\lambda\omega_0 t}{N}\sum_q G(q-p+k,\omega-\omega_0)G(q,\omega-2\omega_0)\right], \quad (2)$$

where $G(k,\omega)$ is the retarded fully renormalized single electron Green's function:

$$G(k,\omega)^{-1}=\omega-\epsilon_k-\Sigma(k,\omega)+i\delta. \quad (3)$$

which will be determined self-consistently. The NCA approach amounts to compute Σ by retaining only the 1 in the square brackets of eq. (2). NCA is formally similar to the ME approximation for metals but it has to be stressed that Migdal criterion has no sense in the case of only one electron having a vanishingly small Fermi surface. The VCA is given by the inclusion also of the second term in square brackets of eq.(2) which represents the first vertex correction. This approach is formally similar to the approximation scheme used in the formulation of the non-adiabatic theory of superconductivity [19]. The present calculations provide therefore also a test of reliability of such an approximation for the one-electron case. The evaluation of self-energy allows to compute the ground state energy given by the lowest energy pole of eq.(3). In the context of dynamical mean-field theory the internal propagators appearing in eq. (2) are averaged over the k-space[15] and the self-energy turns out to be k-independent at any perturbative order.

In fig. 1 we compare the ground-state energy E_0 obtained by ED-1d([2]) with the NCA and

([2]) Different cluster sizes and values of n_{max} have been used in the different physical regimes in

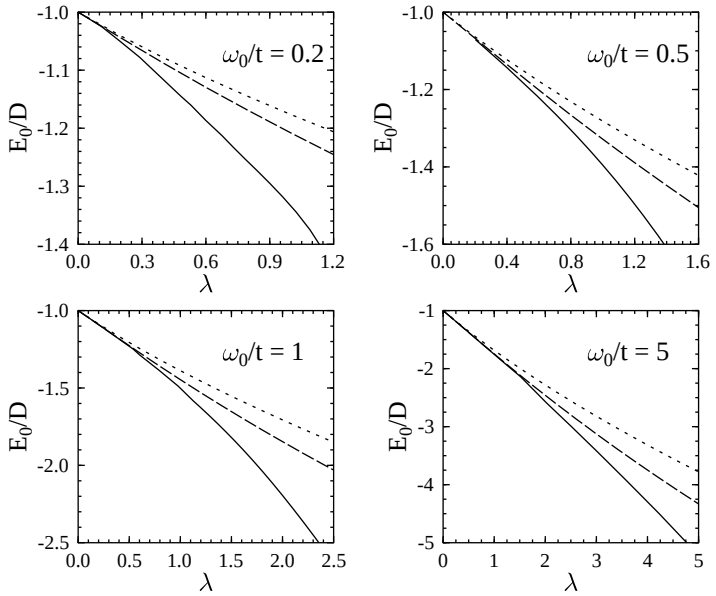

Fig. 1. – Ground state energy results in d=1. The exact diagonalization results are compared with the NCA (short dashed) and VCA (long dashed) calculations.

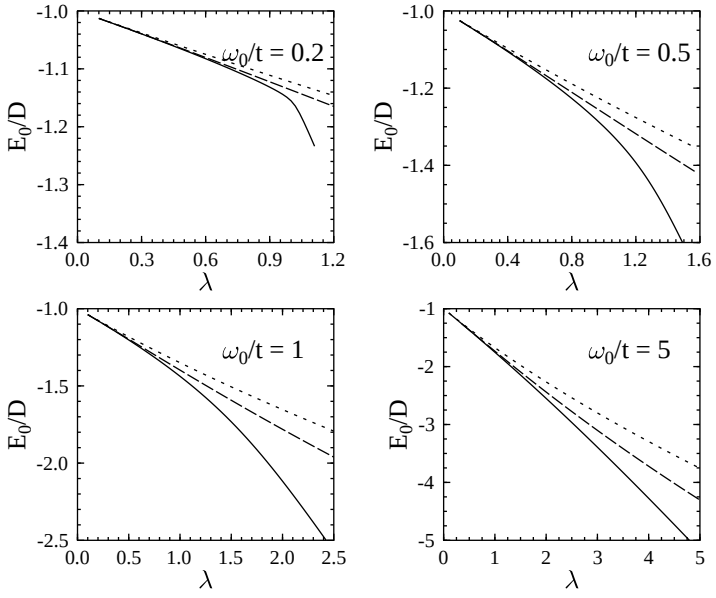

Fig. 2. – Ground state energy results for an infinite coordination lattice. Comparison between dynamical mean field (solid line), NCA (short dashed) and VCA (long dashed).

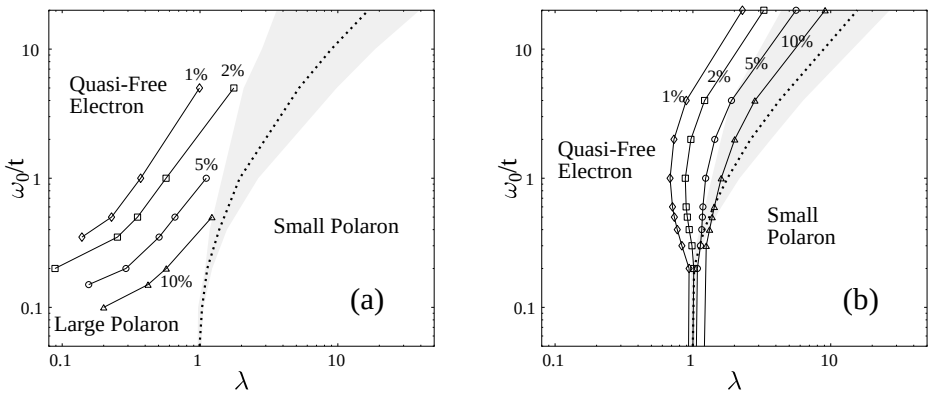

Fig. 3. – Phase diagram in the λ-ω_0/t plane for the one-dimensional (a) and the infinite coordination lattice (b) Holstein model. The dotted line is the polaron crossover value λ_c and the width of the crossover is evidentiated by a shaded area. Notice that the crossover is much broader in the antiadiabatic regime compared to the adiabatic one. The isolines represents the relative difference between the exact and the VCA result for the ground state energy.

VCA results. The same quantities evaluated in the DMFT-3d case are shown in fig. 2. We have chosen the same half-bandwidth D in both DMFT-3d and ED-1d cases.

In the adiabatic regime the agreement of both approximations with exact results strongly depends on the system dimensionality as a result of the different low-energy behaviour of the DOS. In fact, moving from $\omega_0/t = 0.2$ to $\omega_0/t = 0.5$ the agreement of the self-consistent calculations with the exact results is improved for the 1d case (fig. 1) whereas it becomes poorer for the 3d one (fig. 2). Both approximate and exact results tend to become independent on the dimensionality as far as ω_0/t is increased as it is seen from the comparison of fig. 1 and 2 for large ω_0/t. This can be undestood in terms of scattering process which in the anti-adiabatic case will lead electrons through intermediate states out of the band. In this scattering process the system can be thought as a flat band "atomic" system in interaction with high energy phonons. However, the VCA approach represents a significative improvement with respect to the non-crossing approximation for every system dimensionality and over a wide range of parameters. It is also clear from figs. 1 and 2 that both the self-consistent NCA and VCA calculations deviate from the exact results when the crossover towards the small polaron regime is approached.

An exhaustive study of the comparison between the exact results and the VCA approach in the parameter space λ-ω_0/t is shown in figs. 3(a)-(b). We explicitly evaluated both in 1d and 3d the relative difference $\delta E_0 = 2|E_0^{\rm VCA} - E_0^{\rm exact}|/|E_0^{\rm VCA} + E_0^{\rm exact}|$ where $E_0^{\rm exact}$ and $E_0^{\rm VCA}$ are the ground-state energies evaluated by exact techniques and the vertex-corrected approximation, respectively. To analyze the region in the parameter space where the VCA agrees within a given accuracy with the exact results we report lines of constant δE_0.

The agreement between self-consistent approximations and exact results is sensible to system dimensionality. In dimensions larger than two approaching the adiabatic limit and for

order to minimize the finite-size and phonon cut-off effects.

small couplings the electron tends to be free. For this reason self-consistent approximations work well. On the contrary in the adiabatic limit and for d=1 the ground state is a large polaron and self-consistent approximations fail to predict its energy. In general, self-consistent approximations work well outside the polaron region whatever polarons are either small or large. This can be seen directly from figs. 3(a)-(b) where the critical coupling $\lambda_{\rm C}$ of the crossover to small polaron is depicted as a dotted line. The critical coupling λ_c is defined as the value at which dE_0/dg has maximum slope. By Hellmann-Feynman theorem dE_0/dg is just the electron lattice local correlation function $\langle n_i(a_i + a_i^\dagger)\rangle$. In the same figures, we provide also an estimate of the width of the crossover (shaded areas) obtained by looking at the maximum slope of $|\partial^2 E_0/\partial g^2|$. We checked that different criteria, like *e. g.* the effective mass enhancement[15], provide the same qualitative results.

In conclusion, we have shown that the crossover toward the small polaron state depends strongly on the adiabaticity parameter ω_0/t. In the antiadiabatic regime the crossover is ruled by α^2 and it is independent of the system dimensionality whereas in the adiabatic regime the relevant coupling is λ and the details of the crossover depend on the dimensionality. We have also shown that self-consistent calculations provide ground state energies which agree well with exact results in the quasi free electron regime and that such an agreement is increased when vertex corrections are taken into account.

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